Towards High-Fidelity Simulations of EUV Production from Laser-Produced Plasma

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Outline

- Introduction – what can we expect to get from simulations?
- Physical processes important for EUV generation
- Approximations for macroscopic simulations
- Simulating atomic kinetics + radiation transport

How do we improve our simulations and gain confidence in the results?

What should we simulate (and why)?

***for EUV production**

- Explaining general behavior of the EUV-producing system requires
  - Identifying the underlying microphysical processes
  - Evaluating each process (and their interactions) under representative conditions
- A basic understanding is sufficient for:
  - Estimating conversion efficiency (CE) vs. density / temperature / timescale
  - Providing guidance towards optimum conditions
- More details, i.e. simulations, are necessary for:
  - Tracking time evolution of conditions and outputs
- High-fidelity simulations are required for:
  - Predicting behavior in different situations
  - Evaluating effects from asymmetries and shot-to-shot variations

High fidelity requires care in constructing simulations

How reliable are the results?

- Optimizing a system requires predicting the behavior of the system as it evolves through a range of conditions

- Confidence in predictions will be high when
  - Verified by experiment under full range of conditions

    – or –

  - Simulations of microphysical processes and their interactions have been verified
  - Assumptions / approximations remain valid

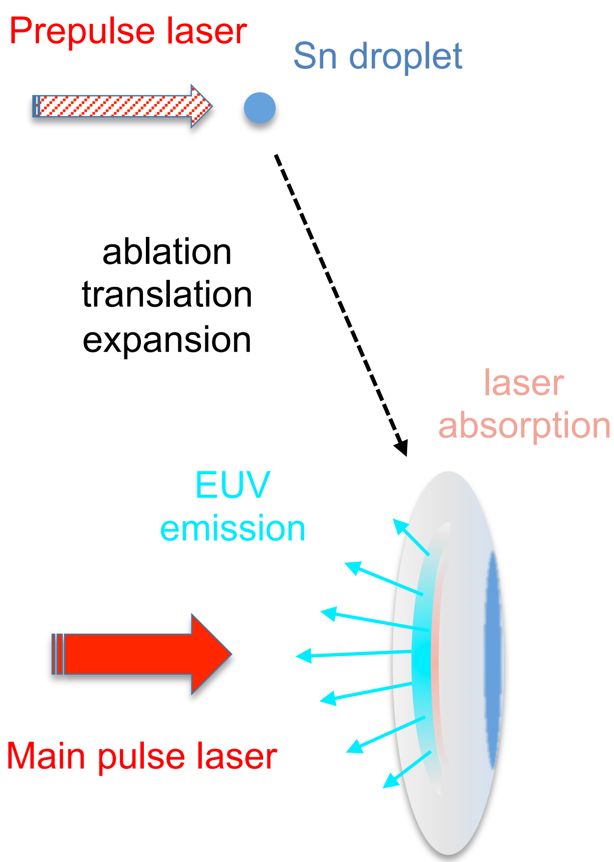
- Getting all the details right is very difficult, but rarely necessary

- Getting the basic descriptions and interactions of the microphysical processes right is critical

Predicting trends does not depend on details, but does depend on valid assumptions and approximations

Physical processes important for EUV generation

- Laser absorption
  - 1 µm (Nd:YAG) or 10 µm (CO_2)
- Mass transport
  - particles or hydrodynamics
- Energy transport via radiation, conduction, advection
- Non-LTE atomic kinetics
- EUV (+ other) radiation production
- Radiation transport



These processes are all interdependent

Simulation at a macroscopic level requires numerous approximations and compromises

- Microphysical processes can be modeled in detail
  - e.g. Maxwell's equations + kinetic (Boltzmann) transport
  - "First principles" is currently <u>not</u> possible for a macroscopic simulation
- Detailed descriptions of physical processes are replaced by derived models
  - Analytical models, tabulated data, "averaged" equations
  - e.g. Laser absorption: ray tracing + inverse bremsstrahlung (low $I\lambda^2$)
  - e.g. Mass transport: hydrodynamics (high collisionality)
  - Derived models can be verified (over a limited range) with detailed simulations
- High fidelity requires
  - Faithful representations of the microphysical interactions
  - Sufficiently high resolution in (space / time / frequency / energy)
  - <u>Controlled</u> approximations to detailed descriptions / numerical treatments

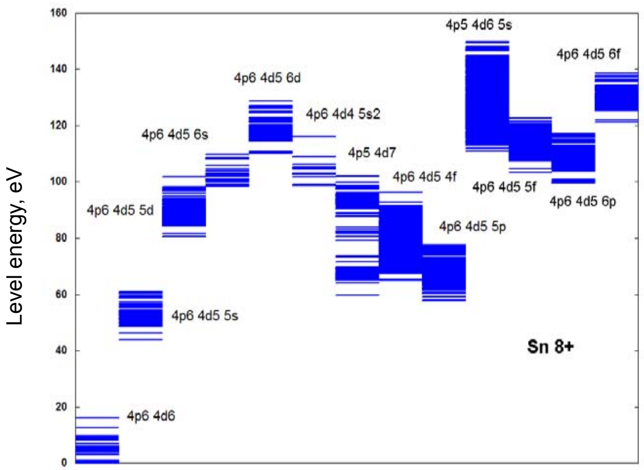
Uncontrolled approximations damage confidence

Atomic physics of EUV-producing Sn

- Transitions producing 13.5 nm radiation:
  4f-4d, 4d-4p, 5d-4p in Sn^{+8-13}
- Data should cover <u>all</u> charge states up to +22
- Atomic levels sufficient to converge populations
  → very large # of levels (>10^{3-5} per charge state)
  → very high resolution needed for spectrum

Approximations:

- Averaged / restricted atomic structure
- Limited configuration interaction (CI)



Koshelev, *et al*, 2006 Source Workshop

- Producing a sufficient amount of accurate data is laborious
- Using the detailed data in a simulation can be just as difficult

Atomic data + NLTE kinetics + radiation transport

- NLTE: Non-Local Thermodynamic Equilibrium
  → excited state populations not in Saha-Boltzmann distribution

- Evaluation of populations:
  Atomic data (energy levels, transition cross-sections)
  \+ Electron and photon distributions
  → atomic populations (time evolution)
  \+ radiative cross-sections
  → radiative emission / absorption
  \+ radiation transport
  → $T_e + T_i$ + photon distribution

iterative procedure

- Populations and radiation are tightly coupled

Coupling NLTE kinetics of detailed atomic levels with high resolution radiation transport presents a <u>major</u> simulation challenge

Incorporating NLTE atomic kinetics into rad-hydro

- Tabulated methods allow inexpensive use of complete atomic data
  - Assumptions / approximations are built into the table
    - NLTE equations solved in steady-state
    - Radiation field specified by assumed conditions
    - Accuracy of current methods is suspect
  - Coupling to other physics is severely limited

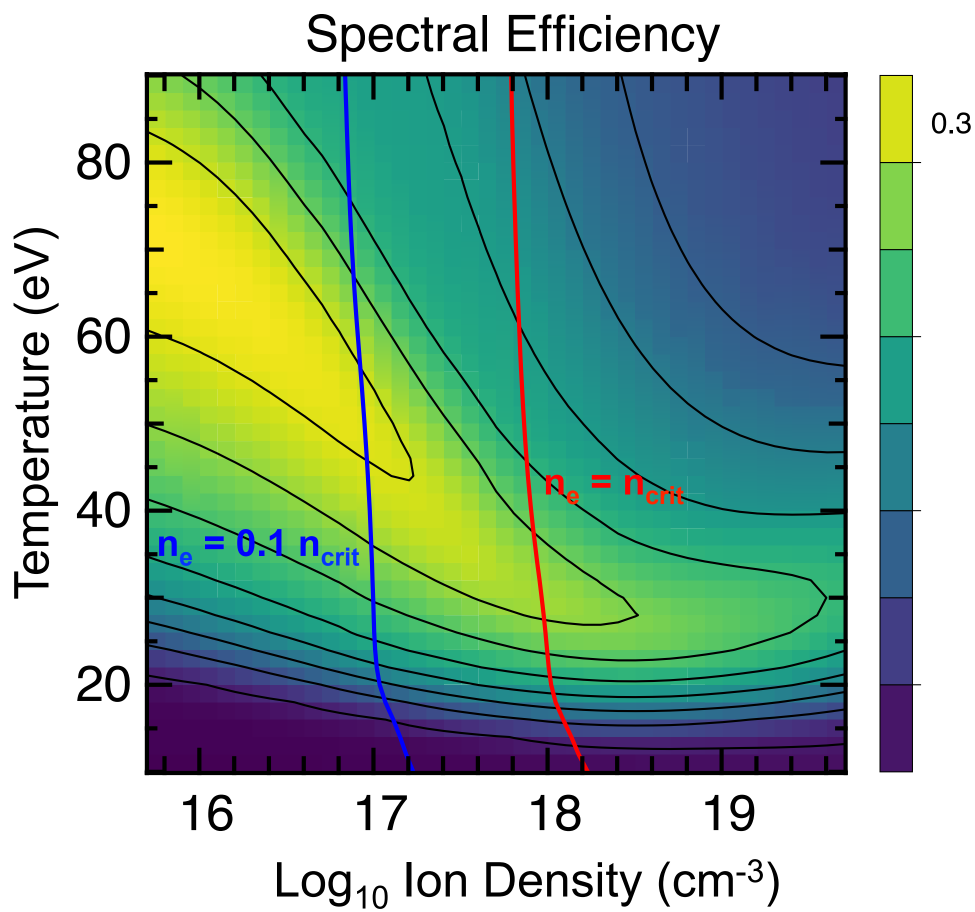
- Inline methods allow full coupling
  - Time-dependent or steady-state evaluation (ref. 2016 workshop)
  - Requires sufficient frequency resolution for energy + ionization balance (and restore higher resolution by postprocessing)
  - BUT: Use of complete atomic data can be prohibitive in both time and memory

- Approximate treatments for inline methods
  - Use of averaged atomic data
  - Reduced coupling to radiation transport

Inline methods can be tested by relaxing approximations

EUV production regime for CO_2 laser (λ = 10.6 μm)

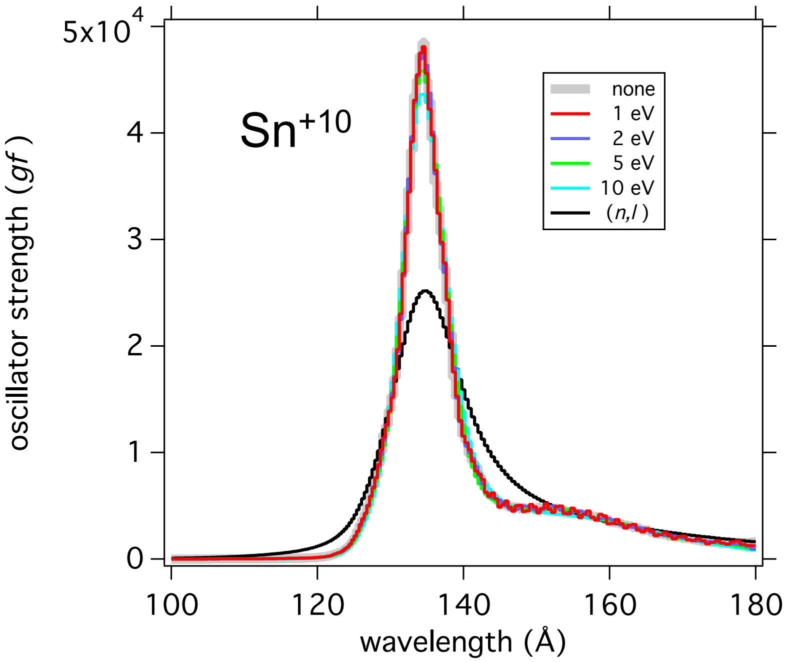
- Spectral efficiency:
  fractional emission in bandpass
- Bandpass emission comes from material with $n_e \sim 0.1 - 1.0\ n_{crit}$
- Assumes steady-state, no radiation field
- Timescales for low n_e, high T_e exceed laser pulse timescale



Critical EUV regime: $n_i \sim 10^{17}$-10^{18} cm^{-3}, $T_e \sim$ 20-60 eV

Reducing the size of the atomic data

- Combine levels by configuration and energy spread
- Averaged transitions between combined levels
- Aim is to maintain <u>oscillator strength distribution</u> in each charge state



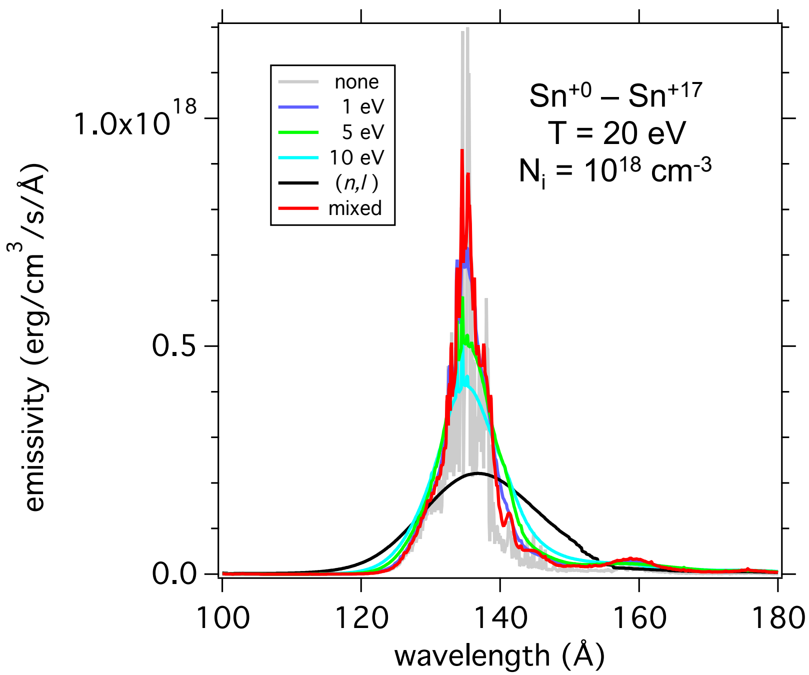
Data from fine-structure model of J. Colgan

averaging	energy levels	transitions
none	141465	3.8e7
1 eV	2397	4.1e5
2 eV	1328	1.5e5
5 eV	603	4.1e4
10 eV	342	1.6e4
(n,l)	59	830

Carefully averaged data maintains the spectral structure

Testing (LTE) radiative emission of averaged models

- Combine levels by configuration and energy spread
- Averaged transitions between combined levels
- Aim is to maintain emission spectrum from each charge state



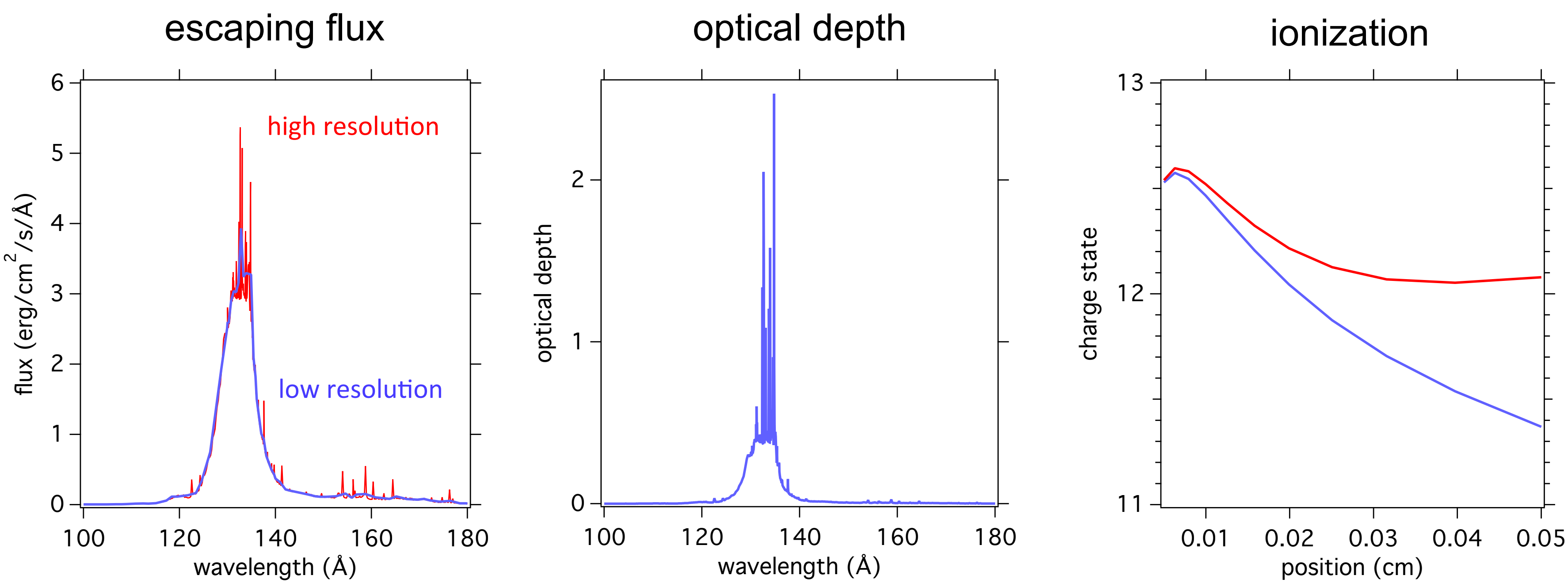
Data from fine-structure model of J. Colgan

averaging	energy levels	transitions
none	1.85e6	4.6e8
1 eV	29668	4.4e6
5 eV	8471	5.2e5
10 eV	5091	2.2e5
(*n*,*l*)	1258	2.0e4
mixed	11072	1.1e6

Carefully averaged data maintains the spectral structure

Testing averaged models with radiation transport

- NLTE atomic kinetics + radiation transport for 1 eV-averaged model
- $T = 30$ eV + maximum $N_i = 10^{18}$ cm^{-3}
- Density profile $N_i \propto r^{-2}$ (fit from rad-hydro simulation)



Bandpass flux is insensitive (<1%) to frequency resolution

Summary

- Reliable simulations require macroscopic models
  - Based on high fidelity microscopic models
  - Constructed with testable, controlled approximations

- Careful averaging of atomic data
  - Maintains spectral characteristics of radiative transitions
  - Allows in-line evaluation with radiation transport
  - Permits development and testing of alternative approaches

High-fidelity predictive simulations are attainable

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